Erratum: Experimental Vibrational Zero-Point Energies: Diatomic Molecules [J. Phys. Chem. Ref. Data 36, 389-397 (2007)]

Cite as: J. Phys. Chem. Ref. Data **38**, 749 (2009); https://doi.org/10.1063/1.3167794 Submitted: 12 June 2009 . Accepted: 12 June 2009 . Published Online: 16 September 2009

Karl K. Irikura





ARTICLES YOU MAY BE INTERESTED IN

Experimental Vibrational Zero-Point Energies: Diatomic Molecules

Journal of Physical and Chemical Reference Data **36**, 389 (2007); https://doi.org/10.1063/1.2436891

Cross Sections for Electron Collisions with Oxygen Molecules
Journal of Physical and Chemical Reference Data 38, 1 (2009); https://doi.org/10.1063/1.3025886

Fundamental Equations of State for Parahydrogen, Normal Hydrogen, and Orthohydrogen Journal of Physical and Chemical Reference Data 38, 721 (2009); https://doi.org/10.1063/1.3160306





Erratum: Experimental Vibrational Zero-Point Energies: Diatomic Molecules [J. Phys. Chem. Ref. Data 36, 389-397 (2007)]

Karl K. Irikura

Chemical and Biochemical Reference Data Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8320, USA

(Received 12 June 2009; accepted 12 June 2009; published online 16 September 2009) [doi:10.1063/1.3167794]

Key words: molecular energetics; uncertainty; vibrational spectroscopy; viscosity; zero-point energy.

There is a typographical error in a state designation for Cl_2^+ on page 390 in the last sentence of Sec. 3. This sentence should read: "For Cl_2^+ , only separate constants for ${}^2\Pi_{3/2g}$ and ${}^2\Pi_{1/2g}$ were reported.⁷"

There is a transcription error for the harmonic frequency (ω_e) of SiF in Table on page 392. The correct entry for SiF in this table should be:

Molecule	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	$lpha_e$	Reference
SiF	857.32507(22)	4.83419(9)	0.019807(16)	0.58125735(21)	0.00503859(39)	84

The transcription error for the harmonic frequency (ω_e) of SiF resulted in an error in the calculated zero point energy (ZPE) for SiF in Table 5 on page 395. The correct entry for SiF in this table should be:

Molecule	State designation	ZPE	$u_{ m stat}$	u_{trunc}
²⁸ Si ¹⁹ F	$^2\Pi$	427.6724(2)	0.00019	0.000021

I thank Dr. Russell D. Johnson III for pointing out these errors.

^{© 2009} by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.